

Endothal  
145-73-3 | DTXSID7024081

Model Performance

Model	Data
-------	------

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

## Model Results

**Predicted value:**  $4.38 \times 10^{-12}$  cm<sup>3</sup>/molecule\*sec

**Global applicability domain:** Inside

**Local applicability domain index:**  $3.71 \times 10^{-1}$

**Confidence level:**  $7.62 \times 10^{-1}$

## Nearest Neighbors from the Training Set

Image not found

Dimethyl adipate

**Measured:**  $8.40 \times 10^{-12}$

**Predicted:**  $6.84 \times 10^{-12}$

Image not found

Dimethyl glutarate

**Measured:**  $3.30 \times 10^{-12}$

**Predicted:**  $3.76 \times 10^{-12}$

Image not found

Dimethyl succinate

**Measured:**  $1.40 \times 10^{-12}$

**Predicted:**  $1.93 \times 10^{-12}$

Image not found

2-Ethoxyethyl isobutyrate

**Measured:**  $1.35 \times 10^{-11}$

**Predicted:**  $1.28 \times 10^{-11}$

Image not found

Ethyl lactate

**Measured:**  $3.90 \times 10^{-12}$

**Predicted:**  $4.80 \times 10^{-12}$